

# Exact quantum algorithms have advantage for almost all Boolean functions

Andris Ambainis<sup>2,3</sup>, Jozef Gruska<sup>1</sup>, Shenggen Zheng<sup>1,\*</sup>

<sup>1</sup>*Faculty of Informatics, Masaryk University, Brno 60200, Czech Republic*

<sup>2</sup>*Faculty of Computing, University of Latvia, Riga, LV-1586, Latvia*

<sup>3</sup>*School of Mathematics, Institute for Advanced Study, Princeton, NJ 08540, USA*

---

## Abstract

It has been proved that almost all  $n$ -bit Boolean functions have *exact classical query complexity*  $n$ . However, the situation seemed to be very different when we deal with *exact quantum query complexity*. In this paper, we prove that almost all  $n$ -bit Boolean functions can be computed by an exact quantum algorithm with less than  $n$  queries. More exactly, we prove that  $\text{AND}_n$  is the only  $n$ -bit Boolean function, up to isomorphism, that requires  $n$  queries.

**Keywords:** Quantum computing, Quantum query complexity, Boolean function, Symmetric Boolean function, Monotone Boolean function, Read-once Boolean function

---

## 1. Introduction

*Quantum query complexity* is the quantum generalization of classical *decision tree complexity*. In this complexity model, an algorithm is charged for “queries” to the input bits, while any intermediate computation is considered as free (see [1]). For many functions one can obtain large quantum speed-ups in this model in the case algorithms are allowed a constant small probability of error (bounded error). As the most famous example, Grover’s algorithm [2] computes the  $n$ -bit OR function with  $O(\sqrt{n})$  queries in the bounded error mode, while any classical (also exact quantum) algorithm needs  $\Omega(n)$  queries. More such cases of polynomial speed-ups are known, see [3–5]. For *partial functions*, even an exponential speed-up is possible, in case quantum resources are used, see [6, 7]. In the bounded-error setting, quantum complexity is now relatively well understood. The model of *exact quantum query complexity*, where the algorithms must output the correct answer with certainty for every input, seems to be more intriguing. It is much more difficult to come up with exact quantum algorithms that outperform, concerning number of queries, classical exact algorithms.

Though for partial functions exact quantum algorithms with exponential speed-up are known (for instance in [8–14]), the results for total functions have been much less spectacular: the best known quantum speed-up was just by a factor of 2 for many years [15, 16]. Recently, in a breakthrough result, Ambainis [17] has presented the first example of a Boolean function  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  for which exact quantum algorithms have superlinear advantage over exact classical algorithms.

In exact classical query complexity (*decision tree complexity*, *deterministic query complexity*) model, almost all  $n$ -bit Boolean functions require  $n$  queries [1]. However, the situation seemed very different for

---

\*Corresponding author.

*E-mail addresses:* andris.ambainis@lu.lv, gruska@fi.muni.cz, zhengshenggen@gmail.com

the case of exact quantum complexity. Montanaro et al. [18] proved that  $\text{AND}_3$  is the only 3-bit Boolean function, up to isomorphism, that requires 3 queries and using the semidefinite programming approach, they numerically<sup>1</sup> demonstrated that all 4-bit Boolean functions, with the exception of functions isomorphic to the  $\text{AND}_4$  function, have exact quantum query algorithms using at most 3 queries. They also listed their numerical results for all symmetric Boolean functions on 5 and 6 bits, up to isomorphism.

In 1998, Beals et al. [19] proved, for any  $n$ , that  $\text{AND}_n$  has exact quantum complexity  $n$ . Since that time it was an interesting problem whether  $\text{AND}_n$  is the only  $n$ -bit Boolean function, up to isomorphism, that has exact quantum complexity  $n$ . In this paper we approve that this is indeed the case. As a corollary we get that almost all  $n$ -bit Boolean functions have exact quantum complexity less than  $n$ .

We prove our main results in four stages. In the first one we give the proof for symmetric Boolean functions, in the second one for monotone Boolean functions and in the third one for the case of read-once Boolean functions. On this basis we prove in the fourth stage the general case. In all four cases proofs used quite different approaches. They are expected to be of a broader interest since all these special classes of Boolean functions are of broad interest.

The paper is organized as follows. In Section 2 we introduce some notation concerning Boolean function and query complexity. In Section 3 we investigate symmetric Boolean functions. In section 4 we investigate monotone Boolean functions. In section 5 we investigate read-once Boolean functions. In Section 6 we prove our main result. Finally, Section 7 contains a conclusion.

## 2. Preliminaries

We introduce some basic needed notation in this section. See also [20, 21] for details on quantum computing and see [1, 19, 22] for more on query complexity models and *multilinear polynomials*.

### 2.1. Boolean functions

An  $n$ -bit Boolean function is a function  $f : \{0, 1\}^n \rightarrow \{0, 1\}$ . We say  $f$  is total if  $f$  is defined on all inputs. For an input  $x \in \{0, 1\}^n$ , we use  $x_i$  to denote its  $i$ -th bit, so  $x = x_1 x_2 \cdots x_n$ . Denote  $[n] = \{1, 2, \dots, n\}$ . For  $i \in [n]$ , we write

$$f_{x_i=b}(x) = f(x_1, \dots, x_{i-1}, b, x_{i+1}, \dots, x_n), \quad (1)$$

which is an  $(n - 1)$  bit Boolean function. For any  $i \in [n]$ , we have

$$f(x) = (1 - x_i)f_{x_i=0}(x) + x_i f_{x_i=1}(x). \quad (2)$$

We say that two Boolean functions  $f$  and  $g$  are *query-isomorphic* (by convenience, isomorphic will mean query-isomorphic in this paper) if they are equal up to negations and permutations of the input variables, and negation of the output variable. This relationship is sometimes known as NPN-equivalence [18].

We will use the sign  $(\neg)$  for a possible negation. For example,  $\text{AND}(\neg x_1, x_2)$  can denote  $x_1 \wedge x_2$  or  $\neg x_1 \wedge x_2$ . We use  $|x|$  to denote the Hamming weight of  $x$  (its number of 1's).

**Definition 1:** We call a Boolean function  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  symmetric if  $f(x)$  depends only on  $|x|$ .

An  $n$ -bit symmetric Boolean function  $f$  can be fully described by a vector  $(b_0, b_1, \dots, b_n) \in \{0, 1\}^{n+1}$ , where  $f(x) = b_{|x|}$ , i.e.  $b_k$  is the value of  $f(x)$  for  $|x| = k$  [23].

---

<sup>1</sup>In their numerical experiments, computation providing correct result with a probability greater than 0.999 is treated as exact.

For  $x, y \in \{0, 1\}^n$ , we will write  $x \preceq y$  if  $x_i \leq y_i$  for all  $i \in [n]$ . We will write  $x \prec y$  if  $x \preceq y$  and  $x \neq y$ .

**Definition 2:** We call a Boolean function  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  monotone if  $f(x) \leq f(y)$  holds whenever  $x \preceq y$ .

Monotonic Boolean functions are precisely those that can be defined by an expression combining the input bits (each of them may appear more than once) using only the operators  $\wedge$  and  $\vee$  (in particular  $\neg$  is forbidden). Monotone Boolean functions have many nice properties. For example they have a unique prime conjunctive normal form (CNF) and a unique prime disjunctive normal form (DNF) in which no negation occurs [24].

Let  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  be a monotone Boolean function,  $f$  has a prime CNF

$$f(x) = \bigwedge_{I \in C} \bigvee_{i \in I} x_i, \quad (3)$$

where  $C$  is the set of some  $I \subseteq [n]$ . Similarly,  $f$  has a prime DNF

$$f(x) = \bigvee_{J \in D} \bigwedge_{j \in J} x_j, \quad (4)$$

where  $D$  is the set of some  $J \subseteq [n]$ .

**Definition 3:** A read-once Boolean function is a Boolean function that can be represented by a Boolean formula in which each variable appears exactly once.

For example  $f(x_1, x_2, x_3) = (x_1 \vee x_2) \wedge (\neg x_3)$  is a 3-bit read-once Boolean function and  $f'(x_1, x_2, x_3) = (x_1 \vee x_2) \wedge (\neg x_1 \vee \neg x_3)$  is not read-once.

A Boolean formula over the standard basis  $\{\wedge, \vee, \neg\}$  can be represented by a binary tree where each internal node is labeled with  $\wedge$  or  $\vee$ , and each leaf is labeled with a literal, that is, a Boolean variable or its negation. The size of a formula is the number of leaves.

**Definition 4:** The formula size of a Boolean function  $f$ , denoted  $L(f)$ , is the size of the smallest formula which computes  $f$ .

A read-once Boolean function is a function  $f$  such that  $L(f) = n$  and  $f$  depends on all of its  $n$  variables.

## 2.2. Exact query complexity models

An exact classical (deterministic) query algorithm for computing a Boolean function  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  can be described by a decision tree. A decision tree  $T$  is a rooted binary tree where each internal vertex has exactly two children, each internal vertex is labeled with a variable  $x_i$  and each leaf is labeled with a value 0 or 1.  $T$  computes a Boolean function  $f$  as follows: Start at the root. If this is a leaf then stop and the output of the tree is the value of the leaf. Otherwise, query the variable  $x_i$  that labels the root. If  $x_i = 0$ , then recursively evaluate the left subtree, if  $x_i = 1$  then recursively evaluate the right subtree. The output of the tree is the value of the leaf that is reached at the end of this process. The depth of  $T$  is the maximal length of a path from the root to a leaf (i.e. the worst-case number of queries used on any input). The *exact classical query complexity* (deterministic query complexity, decision tree complexity)  $D(f)$  is the minimal depth over all decision trees computing  $f$ .

Let  $f : \{0,1\}^n \rightarrow \{0,1\}$  be a Boolean function and  $x = x_1x_2 \cdots x_n$  be an input bit string. Each exact quantum query algorithm for  $f$  works in a Hilbert space with some fixed basis, called standard. It starts in a fixed starting state, then performs on it a sequence of transformations  $U_1, Q, U_2, Q, \dots, U_t, Q, U_{t+1}$ . Unitary transformations  $U_i$  do not depend on the input bits, while  $Q$ , called the *query transformation*, does, in the following way. Each of the basis states corresponds to either one or none of the input bits. If the basis state  $|\psi\rangle$  corresponds to the  $i$ -th input bit, then  $Q|\psi\rangle = (-1)^{x_i}|\psi\rangle$ . If it does not correspond to any input bit, then  $Q$  leaves it unchanged:  $Q|\psi\rangle = |\psi\rangle$ . Finally, the algorithm performs a measurement in the standard basis. Depending on the result of the measurement, the algorithm outputs either 0 or 1 which must be equal to  $f(x)$ . The *exact quantum query complexity*  $Q_E(f)$  is the minimum number of queries used by any quantum algorithm which computes  $f(x)$  exactly for all  $x$ .

Note that if Boolean functions  $f$  and  $g$  are isomorphic, then  $D(f) = D(g)$  and  $Q_E(f) = Q_E(g)$ .

According to Eq. (2), if we query  $x_i$  first, suppose that  $x_i = b$ , then we can compute  $f_{x_i=b}(x)$  further. Therefore, for any  $i \in [n]$ , we have

$$Q_E(f) \leq \max\{Q_E(f_{x_i=0}), Q_E(f_{x_i=1})\} + 1. \quad (5)$$

### 2.3. Some special functions and their exact quantum query complexity

Symmetric, monotone and read-once Boolean functions were well studied in query complexity [1]. The well known Grover's algorithm [2] computes  $\text{OR}_n$ , which is symmetric, monotone and read-once. Read-once functions are also well investigated [25–27].

Some symmetric functions and their exact quantum query complexity that we will refer to in this paper are as follows:

1.  $\text{OR}_n(x) = 1$  iff  $|x| \geq 1$ .  $Q_E(\text{OR}_n) = n$  [19].
2.  $\text{AND}_n(x) = 1$  iff  $|x| = n$ .  $Q_E(\text{AND}_n) = n$  [19].
3.  $\text{PARITY}_n(x) = 1$  iff  $|x|$  is odd.  $Q_E(\text{PARITY}_n) = \lceil \frac{n}{2} \rceil$  [15, 16].
4.  $\text{EXACT}_n^k(x) = 1$  iff  $|x| = k$ .  $Q_E(\text{EXACT}_n^k) = \max\{k, n - k\}$  [28].
5.  $\text{Th}_n^k(x) = 1$  iff  $|x| \geq k$ .  $Q_E(\text{Th}_n^k) = \max\{k, n - k + 1\}$  [28].

$\text{OR}_n$  is isomorphic to  $\text{AND}_n$  since

$$\neg \text{OR}_n(\neg x_1, \neg x_2, \dots, \neg x_n) = \text{AND}_n(x_1, x_2, \dots, x_n). \quad (6)$$

Some other functions and their exact quantum query complexity that we will refer to in this paper are as follows:

1.  $\text{NAE}_n(x) = 1$  iff there exist  $i, j$  such that  $x_i \neq x_j$ .  $Q_E(\text{NAE}_n) \leq n - 1$ .
2.  $f(x_1, x_2, x_3) = x_1 \wedge (x_2 \vee x_3)$ . Its exact quantum query complexity is 2 [18].

It is easy to prove that  $Q_E(\text{NAE}_n) \leq n - 1$  since

$$\text{NAE}_n(x_1, \dots, x_n) = (x_1 \oplus x_2) \vee (x_2 \oplus x_3) \cdots \vee (x_{n-1} \oplus x_n). \quad (7)$$

#### 2.4. Multilinear polynomials

Every Boolean function  $f : \{0,1\}^n \rightarrow \{0,1\}$  has a unique representation as an  $n$ -variate multilinear polynomial over the reals, i.e., there exist real coefficients  $a_S$  such that

$$f(x_1, \dots, x_n) = \sum_{S \subseteq [n]} a_S \prod_{i \in S} x_i. \quad (8)$$

The degree of  $f$  is the degree of its largest monomial:  $\deg(f) = \max\{|S| : a_S \neq 0\}$ .

For example,  $\text{AND}_2(x_1, x_2) = x_1 \cdot x_2$  and  $\text{OR}_2(x_1, x_2) = x_1 + x_2 - x_1 \cdot x_2$ .

$\deg(f)$  gives a lower bound on  $D(f)$ . Indeed, it holds

**Lemma 1.** [1]  $D(f) \geq \deg(f)$ .

### 3. Symmetric Boolean functions

**Theorem 2.** Let  $f : \{0,1\}^n \rightarrow \{0,1\}$  be a symmetric Boolean function.  $Q_E(f) = n$  iff  $f$  is isomorphic to  $\text{AND}_n$ .

*Proof.* If  $f$  is isomorphic to  $\text{AND}_n$ , then  $Q_E(f) = n$  [19].

An  $n$ -bit symmetric Boolean function can be fully described by a vector  $(b_0, b_1, \dots, b_n) \in \{0,1\}^{n+1}$ , where  $f(x) = b_{|x|}$ , i.e.  $b_k$  is the value of  $f(x)$  for  $|x| = k$ .

Table 1: Exact quantum query complexity for 3-bit symmetric functions.

$(b_0, b_1, b_2, b_3)$	Type of function	Query complexity
0 0 0 0	Constant function	0
0 0 0 1	$\text{AND}_3$	3
0 0 1 0	$\text{EXACT}_3^2$	2
0 0 1 1	$\text{Th}_3^2$	2
0 1 0 0	$\text{EXACT}_3^1$	2
0 1 0 1	$\text{PARITY}_3$	2
0 1 1 0	$\text{NAE}_3$	2
0 1 1 1	Isomorphic to $\text{AND}_3$	3
1 0 0 0	Isomorphic to $\text{AND}_3$	3
1 0 0 1	Isomorphic to $\text{NAE}_3$	2
1 0 1 0	Isomorphic to $\text{PARITY}_3$	2
1 0 1 1	Isomorphic to $\text{EXACT}_3^1$	2
1 1 0 0	Isomorphic to $\text{Th}_3^2$	2
1 1 0 1	Isomorphic to $\text{EXACT}_3^2$	2
1 1 1 0	Isomorphic to $\text{AND}_3$	3
1 1 1 1	Constant function	0

Table 1 contains all 3-bit Boolean functions and their exact quantum query complexity. Four 3-bit Boolean functions that achieve 3 queries are those that can be described by one of the following vectors:  $(0, 0, 0, 1)$ ,  $(0, 1, 1, 1)$ ,  $(1, 0, 0, 0)$ ,  $(1, 1, 1, 0)$ . They are isomorphic to  $\text{AND}_3$ .

We claim that only  $n$ -bit Boolean functions that can be described by one of the following vectors  $(0, \dots, 0, 1), (0, 1, \dots, 1), (1, 0, \dots, 0), (1, \dots, 1, 0)$ , which are isomorphisms of  $\text{AND}_n$ , that can achieve  $n$  queries. We prove this claim by an induction on  $n$  as follows:

**BASIS:** The result holds clearly for  $n = 3$ .

**INDUCTION:** Suppose the result holds for  $n = k$  ( $\geq 3$ ). We will prove that the result holds also for  $n = k + 1$ . We use vector  $(b_0, b_1, \dots, b_k, b_{k+1})$  to describe the function  $f(x_1, \dots, x_k, x_{k+1})$ . Since

$$Q_E(f) \leq \max\{Q_E(f_{x_1=0}), Q_E(f_{x_1=1})\} + 1, \quad (9)$$

we just need to consider the case that at least one of the functions  $f_{x_1=0}$  and  $f_{x_1=1}$  is isomorphic to  $\text{AND}_k$ . For other cases we have  $Q_E(f) < k + 1$ .

Table 2: Exact quantum query complexity for  $(k + 1)$ -bit symmetric Boolean functions.

$b_0 b_1 \dots, b_k, b_{k+1}$	Type of function	Query complexity
$(0,  0, \dots, 0, 1)$	$\text{AND}_{k+1}$	$k + 1$
$(0,  0, 1, \dots, 1)$	$\text{Th}_{k+1}^2$	$k$
$(0,  1, 0, \dots, 0)$	$\text{EXACT}_{k+1}^1$	$k$
$(0,  1, \dots, 1, 0)$	$\text{NAE}_{k+1}$	$< k + 1$
$(1,  0, \dots, 0, 1)$	Isomorphic to $\text{NAE}_{k+1}$	$< k + 1$
$(1,  0, 1, \dots, 1)$	Isomorphic to $\text{EXACT}_{k+1}^1$	$k$
$(1,  1, 0, \dots, 0)$	Isomorphic to $\text{Th}_{k+1}^2$	$k$
$(1,  1, \dots, 1, 0)$	Isomorphic to $\text{AND}_{k+1}$	$k + 1$
$(0, \dots, 0, 1,  0)$	$\text{EXACT}_{k+1}^k$	$k$
$(0, 1, \dots, 1,  0)$	$\text{NAE}_{k+1}$	$< k + 1$
$(1, 0, \dots, 0,  0)$	Isomorphic to $\text{AND}_{k+1}$	$k + 1$
$(1, \dots, 1, 0,  0)$	Isomorphic to $\text{Th}_{k+1}^k$	$k$
$(0, \dots, 0, 1,  1)$	$\text{Th}_{k+1}^k$	$k$
$(0, 1, \dots, 1,  1)$	Isomorphic to $\text{AND}_{k+1}$	$k + 1$
$(1, 0, \dots, 0,  1)$	Isomorphic to $\text{NAE}_{k+1}$	$< k + 1$
$(1, \dots, 1, 0,  1)$	Isomorphic to $\text{EXACT}_{k+1}^k$	$k$

There are three cases we have to consider according to the value of  $b$ .

**Case 1**  $b = (0, \dots, 0, 1)$ . In this case  $f = \text{AND}_{k+1}$ .

**Case 2**  $b = (1, 0, \dots, 0)$ . In this case  $f$  is isomorphic to  $\text{AND}_{k+1}$ .

**Case 3** Otherwise,  $f_{x_1=0}$  can be described by the vector  $(b_0, b_1, \dots, b_k)$  and  $f_{x_1=1}$  can be described by the vector  $(b_1, \dots, b_k, b_{k+1})$ . Thus we just need to consider Boolean functions that can be described by vector  $b = (b_0, b_1, \dots, b_k, b_{k+1})$  such that one of the following vectors

$$(\overbrace{0, \dots, 0}^k, 1), (0, \overbrace{1, \dots, 1}^k), (1, \overbrace{0, \dots, 0}^k), (\overbrace{1, \dots, 1}^k, 0) \quad (10)$$

is its prefix or suffix<sup>2</sup>. There are 16 such Boolean functions and their query complexity are listed in Table 2.

<sup>2</sup>Let  $b = (b_0, b_1, \dots, b_{k+1})$ . We say that  $(b_0, \dots, b_k)$  is a prefix of  $b$  and  $(b_1, \dots, b_{k+1})$  a suffix of  $b$ .

According to Table 2, only  $(k+1)$ -bit Boolean functions which are isomorphic to  $\text{AND}_{k+1}$  require  $k+1$  queries. Thus, the theorem has been proved.  $\square$

It is mentioned in [18, 29] that all non-constant  $n$ -bit symmetric Boolean functions have exact classical complexity  $n$ . We give now a rigorous proof of that.

**Theorem 3.** *If  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  is a non-constant symmetric function, then  $D(f) = n$ .*

*Proof.* Suppose  $f$  can be described by the vector  $(b_0, b_1, \dots, b_n) \in \{0, 1\}^{n+1}$ . Since  $f$  is non-constant, there exists a  $k \in [n]$  such that  $b_{k-1} \neq b_k$ . If the first  $k-1$  queries return  $x_i = 1$  and the next  $n-k$  queries return  $x_i = 0$ , then we will need to query the last variable as well.  $\square$

#### 4. Monotone Boolean functions

**Theorem 4.** *Let  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  be a monotone Boolean function.  $Q_E(f) = n$  iff  $f$  is isomorphic to  $\text{AND}_n$ .*

*Proof.* Obviously,  $\text{AND}_n(x)$  and  $\text{OR}_n(x)$  are the only two  $n$ -bit monotone Boolean functions that are isomorphic to  $\text{AND}_n(x)$ . If  $f$  is isomorphic to  $\text{AND}_n(x)$ , then  $Q_E(f) = n$  [19]. We prove the other direction by an induction on  $n$ .

**BASIS:** Case  $n = 2$ ,  $\text{AND}_2(x_1, x_2)$  is the only 2-bit function, up to isomorphism, that requires 2 queries. Therefore the result holds for  $n = 2$ .

**INDUCTION:** Suppose the result holds for all  $n \leq k$ , we prove that the result holds also for  $n = k+1$  in the following way.

For any  $i \in [k+1]$ , if  $Q_E(f_{x_i=0}) < k$  and  $Q_E(f_{x_i=1}) < k$ , then  $Q_E(f) \leq \max\{Q_E(f_{x_i=0}), Q_E(f_{x_i=1})\} + 1 < k+1$ . Therefore, we need to consider only the case that at least one of functions  $f_{x_i=0}$  and  $f_{x_i=1}$  requires  $k$  queries. There are two such cases:

**Case 1:**  $Q_E(f_{x_1=1}) = k$ . According to the assumption,  $f_{x_1=1}$  is isomorphic to  $\text{AND}_k$ . There are now two subcases to consider:

**Case 1a:**  $f_{x_1=1}(x) = \text{OR}_k(x_2, \dots, x_{k+1}) = \text{OR}_k(x_{-1})$  (For convenience, we write  $x_{-i} = x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{k+1}$ ). Let us consider the CNF of  $f$ :

$$f(x) = \bigwedge_{I \in C} \bigvee_{i \in I} x_i = \left( \bigwedge_{I \in C, 1 \in I} \bigvee_{i \in I} x_i \right) \wedge \left( \bigwedge_{I \in C, 1 \notin I} \bigvee_{i \in I} x_i \right). \quad (11)$$

Therefore,

$$f(x) = (x_1 \vee g_1(x_{-1})) \wedge \text{OR}_k(x_{-1}), \quad (12)$$

where  $x_1 \vee g_1(x_{-1}) = \left( \bigwedge_{I \in C, 1 \in I} \bigvee_{i \in I} x_i \right)$  and  $g_1$  is also a monotone function. So we have  $f(x) = 1$  for any  $x$  such that  $10 \cdots 0 \prec x$  and  $f(x) = 0$  for any  $x$  such that  $x \preceq 10 \cdots 0$ .

Let us consider now two subcases. Namely  $f_{x_2=1}$  and  $f_{x_2=0}$ . Since  $10 \cdots 0 \preceq 10 \cdots 0$ , we have  $f(10 \cdots 0) = 0$  and  $f_{x_2=0}(x) \neq \text{OR}_k(x_{-2})$ . Since  $10 \cdots 0 \prec 1010 \cdots 0$ , we have  $f(1010 \cdots 0) = 1$  and  $f_{x_2=0}(x) \neq \text{AND}_k(x_{-2})$ . Now we have  $Q_E(f_{x_2=0}) < k$  and therefore  $Q_E(f_{x_2=1}) = k$ . Since  $10 \cdots 0 \prec 110 \cdots 0$ , we have  $f(110 \cdots 0) = 1$  and  $f_{x_2=1}(x) \neq \text{AND}_k(x_{-2})$ . Therefore,  $f_{x_2=1}(x) = \text{OR}_k(x_{-2})$ . Using a similar argument, we can prove that for any  $i \geq 2$ ,  $f_{x_i=1}(x) = \text{OR}_k(x_{-i})$ . Hence, for any  $i \in [k+1]$ , we have

$$f(x) = (x_i \vee g_i(x_{-i})) \wedge \text{OR}_k(x_{-i}). \quad (13)$$

So  $f(x) = 1$  for any  $x$  such that  $y \prec x$  and  $f(x) = 0$  for any  $x$  such that  $x \preceq y$ , where  $y_i = 1$  and  $y_j = 0$  for any  $j \neq i$ . It is not hard to see that in this case  $f(x) = \text{Th}_{k+1}^2(x)$  and therefore  $Q_E(f) = k$ .

**Case 1b:**  $f_{x_1=1}(x) = \text{AND}_k(x_{-1})$ . Let us consider the CNF of  $f$ . We have,

$$f(x) = (x_1 \vee g'(x_{-1})) \wedge \text{AND}_k(x_{-1}), \quad (14)$$

where  $g'(x_{-1})$  is also a monotone Boolean function.

If  $g'$  is a constant function and  $g'(x_{-1}) = 0$ , we have  $f(x) = \text{AND}_{k+1}(x_1 x_2, \dots, x_{k+1})$  and  $Q_E(f) = k+1$ . Otherwise,  $\text{AND}_k(x_{-1}) \leq g'(x_{-1})$ , then  $f(x) = \text{AND}_k(x_{-1})$  and therefore  $Q_E(f) = k$ .

**Case 2:**  $Q_E(f_{x_1=0}) = k$ . There are again two subcases:

**Case 2a:**  $f_{x_1=0}(x) = \text{OR}_k(x_{-1})$ . Let us consider the DNF of  $f$ :

$$f(x) = \bigvee_{I \in D} \bigwedge_{i \in I} x_i = \left( \bigvee_{I \in D, 1 \in I} \bigwedge_{i \in I} x_i \right) \vee \left( \bigvee_{I \in D, 1 \notin I} \bigwedge_{i \in I} x_i \right). \quad (15)$$

We have

$$f(x) = (x_1 \wedge h'(x_{-1})) \vee \text{OR}_{n-1}(x_{-1}), \quad (16)$$

where  $h'$  is a monotone Boolean function. If  $h'$  is a constant function and  $h'(x_{-1}) = 1$ , then  $f(x) = \text{OR}_{k+1}(x_1 x_2, \dots, x_{k+1})$  and  $Q_E(f) = k+1$ . Otherwise  $h'(x_{-1}) \leq \text{OR}_k(x_{-1})$  and therefore  $f(x) = \text{OR}_k(x_{-1})$  and  $Q_E(f) = k$ .

**Case 2b:**  $f_{x_1=0}(x) = \text{AND}_k(x_{-1})$ . Let us consider the DNF of  $f$ . It has the form

$$f(x) = (x_1 \wedge h_1(x_{-1})) \vee \text{AND}_k(x_{-1}), \quad (17)$$

where  $h_1(x_{-1})$  is also a monotone Boolean function. Therefore  $f(x) = 1$  for any  $x$  such that  $01 \dots 1 \preceq x$  and  $f(x) = 0$  for any  $x$  such that  $x \prec 01 \dots 1$ .

Let us consider now two subcases:  $f_{x_2=1}$  and  $f_{x_2=0}$ . Since  $0110 \dots 0 \prec 01 \dots 1$ , we have  $f(0110 \dots 0) = 0$  and  $f_{x_2=1}(x) \neq \text{OR}_k(x_{-2})$ . Since  $01 \dots 1 \preceq 01 \dots 1$ , we have  $f(01 \dots 1) = 1$  and  $f_{x_2=1}(x) \neq \text{AND}_k(x_{-2})$ . Therefore we have  $Q_E(f_{x_2=1}) < k$  and  $Q_E(f_{x_2=0}) = k$ . Since  $0010 \dots 0 \prec 01 \dots 1$ , we have  $f(0010 \dots 0) = 0$  and  $f_{x_2=0}(x) \neq \text{OR}_k(x_{-2})$ . Therefore,  $f_{x_2=0}(x) = \text{AND}_k(x_{-2})$ . Using a similar argument, we can prove that for any  $i \geq 2$ ,  $f_{x_i=0}(x) = \text{AND}_k(x_{-i})$ . Hence, for any  $i \in [k+1]$ , we have

$$f(x) = (x_i \wedge h_i(x_{-i})) \vee \text{AND}_k(x_{-i}). \quad (18)$$

Therefore  $f(x) = 1$  for any  $x$  such that  $y \preceq x$  and  $f(x) = 0$  for any  $x$  such that  $x \prec y$ , where  $y_i = 0$  and  $y_j = 1$  for any  $j \neq i$ . It is now not hard to show that  $f(x) = \text{Th}_{k+1}^k$  and  $Q_E(f) = k$ .

Therefore, the theorem has been proved.  $\square$

## 5. Read-once Boolean functions

**Theorem 5.** *If  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  is a read-once Boolean function, then  $Q_E(f) = n$  iff  $f$  is isomorphic to  $\text{AND}_n$ .*

*Proof.* If  $f$  is isomorphic to  $\text{AND}_n$ , then  $Q_E(f) = n$  [19]. We prove the other direction as follows.

Since  $f$  is a read-once Boolean function,  $f$  depends on all  $n$  variables and  $L(f) = n$ , i.e each  $(\neg)x_i$  labels once and only once a leaf variable, where  $(\neg)$  denotes a possible negation. We prove the result by an induction.



**BASIS:**  $\text{AND}_3(x_1, x_2, x_3)$  is the only 3-bit Boolean function, up to isomorphism, that requires 3 quantum queries [18]. Therefore the result holds for  $n = 3$ .

**INDUCTION:** We will suppose the result holds for all  $n \leq k$  ( $k \geq 3$ ) and we will prove that the result holds also for all  $n \leq k + 1$ .

Suppose the root of a formula  $F$  is labeled with  $\wedge$ . Without loss of generality, we assume that there exist Boolean functions  $g : \{0, 1\}^p \rightarrow \{0, 1\}$  and  $h : \{0, 1\}^q \rightarrow \{0, 1\}$  such that  $f(x) = g(y) \wedge h(z)$  and  $p + q = k + 1$ , where  $x = yz$ . Since  $f$  depends on all  $k + 1$  variables and  $L(f) = k + 1$ , we have  $L(g) = p$  and  $L(h) = q$ , where  $g$  depends on all  $p$  variables and  $h$  depends on all  $q$  variables. If  $Q_E(g) < p$  or  $Q_E(h) < q$ , then  $Q_E(f) \leq Q_E(g) + Q_E(h) < k + 1$ . Now suppose  $Q_E(g) = p$  and  $Q_E(h) = q$ . According to the assumption,  $g$  is isomorphic to  $\text{AND}_p$  and  $h$  is isomorphic to  $\text{AND}_q$ . There are therefore the following four cases to consider.

**Case 1:**  $g(y) = \text{AND}_p((\neg)x_1, \dots, (\neg)x_p)$  and  $h(z) = \text{AND}_q((\neg)x_{p+1}, \dots, (\neg)x_{k+1})$ . Then  $f$  is isomorphic to  $\text{AND}_{k+1}$  and therefore  $Q_E(f) = k + 1$ .

**Case 2:**  $g(y) = \text{OR}_p((\neg)x_1, \dots, (\neg)x_p)$  and  $h(z) = \text{OR}_q((\neg)x_{p+1}, \dots, (\neg)x_{k+1})$ . Therefore

$$f(x) = \text{OR}_p((\neg)x_1, \dots, (\neg)x_p) \wedge \text{OR}_q((\neg)x_{p+1}, \dots, (\neg)x_{k+1}). \quad (19)$$

Without loss of generality, we suppose that  $f(x) = \text{OR}_p(x_1, \dots, x_p) \wedge \text{OR}_q(x_{p+1}, \dots, x_{k+1})$ . Since  $p + k - p + 1 = k + 1 > 3$ , we have  $p \geq 2$  or  $k - p + 1 \geq 2$ . Without loss of generality, we assume that  $k - p + 1 \geq 2$ . Let us query  $x_2$  to  $x_{k-1}$  first.

- 1) If  $x_i = 1$  for some  $2 \leq i \leq p$  and  $x_j = 1$  for some  $p + 1 \leq j \leq k - 1$ , then  $f_{x_2 \dots x_{k-1}}(x) = 1$ .
- 2) If  $x_i = 1$  for some  $2 \leq i \leq p$  and  $x_{p+1} = \dots = x_{k-1} = 0$ , then  $f_{x_2 \dots x_{k-1}}(x) = \text{OR}_2(x_k, x_{k+1})$ .
- 3) If  $x_2 = \dots = x_p = 0$  and  $x_i = 1$  for some  $p + 1 \leq i \leq k - 1$ , then  $f_{x_2 \dots x_{k-1}}(x) = x_1$ .
- 4) Otherwise,  $x_2 = \dots = x_{k-1} = 0$  and therefore  $f_{x_2 \dots x_{k-1}}(x) = x_1 \wedge (x_k \vee x_{k+1})$  and  $Q_E(f_{x_2 \dots x_{k-1}}) = 2$ .

Therefore  $Q_E(f) \leq k - 2 + 2 < k + 1$ .

**Case 3:**  $g(y) = \text{AND}_p((\neg)x_1, \dots, (\neg)x_p)$  and  $h(z) = \text{OR}_q((\neg)x_{p+1}, \dots, (\neg)x_{k+1})$ . Therefore  $f(x) = \text{AND}_p((\neg)x_1, \dots, (\neg)x_p) \wedge \text{OR}_q((\neg)x_{p+1}, \dots, (\neg)x_{k+1})$ . Without loss of generality, we can now suppose that

$$f(x) = \text{AND}_p(x_1, \dots, x_p) \wedge \text{OR}_q(x_{p+1}, \dots, x_{k+1}). \quad (20)$$

If  $p = k$ , then  $f = \text{AND}_{k+1}$  and  $Q_E(f) = k + 1$ . Now we consider the case  $p < k$ . Let us query  $x_2$  to  $x_{k-1}$  first.

- 1) If  $x_2 \dots x_p \neq 1 \dots 1$ , then  $f(x) = 0$ .
- 2) If  $x_2 \dots x_p = 1 \dots 1$  and  $x_{p+1} \dots x_{k-1} \neq 0 \dots 0$ , then  $f_{x_2 \dots x_{k-1}}(x) = x_1$ .
- 3) If  $x_2 \dots x_p = 1 \dots 1$  and  $x_{p+1} \dots x_{k-1} = 0 \dots 0$ , then  $f_{x_2 \dots x_{k-1}}(x) = x_1 \wedge (x_k \vee x_{k+1})$  and  $Q_E(f_{x_2 \dots x_{k-1}}) = 2$ .

Therefore  $Q_E(f) \leq k - 2 + 2 < k + 1$ .

**Case 4:**  $g(y) = \text{OR}_p((\neg)x_1, \dots, (\neg)x_p)$  and  $h(z) = \text{AND}_q((\neg)x_{p+1}, \dots, (\neg)x_{k+1})$ . This case is analogous to the **Case 3**.

Symmetrically, we can consider the case that the root of the formula  $F$  is labeled with  $\vee$ . In this case, we will need to deal with functions with the same structure of  $f(x_1, x_2, x_3) = x_1 \vee (x_2 \wedge x_3)$ , which is isomorphic to  $x_1 \wedge (x_2 \vee x_3)$ . We omit the details here.  $\square$

It is mentioned in [27] that all  $n$ -bit read-once Boolean functions have exact classical quantum complexity  $n$ . We give now a rigorous proof of that:

**Theorem 6.** *If  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  is a read-once Boolean function, then  $D(f) = n$ .*

*Proof.* Let us consider the multilinear polynomial representation of  $f$ . It is easy to prove by induction that  $\deg(f) = n$  and there is just one monomial of  $f$  of the degree  $n$ .

**BASIS:** If  $n = 1$ , then  $f(x) = (\neg)x_1$ . Therefore,  $\deg(f) = 1$ .

**INDUCTION:** Suppose the result holds for all  $n \leq k$ , we will prove the result holds for all  $n \leq k + 1$ .

Without loss of generality, let us assume that there exists an  $i \in [n]$  such that

$$f(x_1, \dots, x_{k+1}) = g(x_1, \dots, x_i) \wedge h(x_{i+1}, \dots, x_{k+1}) \quad (21)$$

or

$$f(x_1, \dots, x_{k+1}) = g(x_1, \dots, x_i) \vee h(x_{i+1}, \dots, x_{k+1}), \quad (22)$$

where  $L(g) = i$ ,  $L(h) = k + 1 - i$ ,  $g$  and  $h$  depend on all their variables. According to assumption of the theorem, we have  $\deg(g) = i$  and  $g(x_1, \dots, x_i) = (\pm) \prod_{j=1}^i (\neg)x_j + p(x_1, \dots, x_i)$  where  $\deg(p) < i$ , and  $\deg(h) = k + 1 - i$  and  $h(x_{i+1}, \dots, x_{k+1}) = (\pm) \prod_{j=i+1}^{k+1} (\neg)x_j + q(x_{i+1}, \dots, x_{k+1})$  where  $\deg(q) < k + 1 - i$ .

Since

$$f(x_1, \dots, x_{k+1}) = g(x_1, \dots, x_i) \wedge h(x_{i+1}, \dots, x_{k+1}) = g \cdot h \quad (23)$$

and

$$f(x_1, \dots, x_{k+1}) = g(x_1, \dots, x_i) \vee h(x_{i+1}, \dots, x_{k+1}) = g + h - g \cdot h. \quad (24)$$

Therefore  $\deg(f) = k + 1$  and there is just one monomial of  $f$  of the degree  $k + 1$ .

According to Lemma 1,  $D(f) \geq \deg(f) = n$ . Thus,  $D(f) = n$ .  $\square$

## 6. General $n$ -bit Boolean functions

In this section we prove our main result. Without explicitly pointed out,  $n > 3$  in this section.

If  $f$  is an  $n$ -bit Boolean function that is isomorphic to  $\text{AND}_n$ , then there must exist  $b = b_1 \dots b_n \in \{0, 1\}^n$  such that every  $f_{x_i=b_i}$  is equivalent to  $\text{AND}_{n-1}$  ( $\text{OR}_{n-1}$ ) up to some negations of variables. Moreover  $b$  has to be unique. For example, if  $f(x) = \text{OR}_n(x_1, x_2, \dots, x_n)$ , then we have  $f_{x_i=0}(x) = \text{OR}_{n-1}(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$  for  $i \in [n]$  and  $b = 0 \dots 0$ .

For an  $n$ -bit Boolean function  $f$  that has exact quantum query complexity  $n$ , we prove the following lemma.

**Lemma 7.** *Suppose that  $\text{AND}_{n-1}$  is the only  $(n-1)$ -bit Boolean function, up to isomorphism, has exact quantum query complexity  $n - 1$ . Let  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  be an  $n$ -bit Boolean function that has exact quantum query complexity  $n$ . There exists one and only one  $b = b_1 \dots b_n \in \{0, 1\}^n$  for every  $i \in [n]$  such that  $f_{x_i=b_i}$  is equivalent to  $\text{AND}_{n-1}$  ( $\text{OR}_{n-1}$ ) up to some negations of the variables.*

**Proof:** In order to prove this lemma, we study some properties of exact quantum query complexity of Boolean functions. According to Eq. (5), we have the following lemma:

**Lemma 8.** Let  $f : \{0,1\}^n \rightarrow \{0,1\}$  be a Boolean function. If there exists an  $i \in [n]$  such that both  $Q_E(f_{x_i=0}) < n-1$  and  $Q_E(f_{x_i=1}) < n-1$ , then  $Q_E(f) < n$ .

We know from [18] that  $\text{AND}_3$  is the only 3-bit Boolean function, up to isomorphism, that has exact quantum query complexity 3. For any 4-bit function  $f$ , if there exists  $i \in [4]$  such that neither  $f_{x_i=0}$  nor  $f_{x_i=1}$  is isomorphic to  $\text{AND}_{n-1}$ , then  $Q_E(f) < 4$ .

**Lemma 9.** Let  $f : \{0,1\}^n \rightarrow \{0,1\}$  be a Boolean function. If there exists an  $i \in [n]$  such that both  $f_{x_i=0}$  and  $f_{x_i=1}$  are isomorphic to  $\text{AND}_{n-1}$ , then  $Q_E(f) < n$ .

**Proof:** Without loss of generality, we can assume that  $i = 1$ . According to Eq. (2), we have

$$f(x) = (\neg x_1 \wedge f_{x_1=0}(x_2, \dots, x_n)) \vee (x_1 \wedge f_{x_1=1}(x_2, \dots, x_n)). \quad (25)$$

Suppose that at least one of the functions  $f_{x_1=0}$  and  $f_{x_1=1}$  is equivalent to  $\text{AND}_{n-1}$  up to some negations of the variables. Without loss of generality, we will now assume that  $f_{x_1=1}(x) = \text{AND}_{n-1}(x_2, \dots, x_n)$ . To prove the theorem, we consider two cases.

**Case 1:**  $f_{x_1=0}(x) = \text{AND}_{n-1}((\neg)x_2, \dots, (\neg)x_n)$ . In this case we have two subcases.

**Case 1a:**  $f_{x_1=0}(x) = \text{AND}_{n-1}(\neg x_2, \dots, \neg x_n)$ . We have

$$f(x) = \text{AND}_n(\neg x_1, \neg x_2, \dots, \neg x_n) \vee \text{AND}_n(x_1, x_2, \dots, x_n) = \neg \text{NAE}(x_1, x_2, \dots, x_n).$$

Therefore,  $Q_E(f) < n$ .

**Case 1b:**  $f_{x_1=0}(x) \neq \text{AND}_{n-1}(\neg x_2, \dots, \neg x_n)$ . Without loss of generality, we can suppose that there exists a  $k \in \{2, \dots, n-1\}$  such that  $f_{x_1=0}(x) = \text{AND}_{n-1}(\neg x_2, \dots, \neg x_k, x_{k+1}, \dots, x_n)$ . Then

$$\begin{aligned} f(x) &= \text{AND}_n(\neg x_1, \dots, \neg x_k, x_{k+1}, \dots, x_n) \vee \text{AND}_n(x_1, x_2, \dots, x_n) \\ &= (\text{AND}_k(\neg x_1, \dots, \neg x_k) \vee \text{AND}_k(x_1, \dots, x_k)) \wedge \text{AND}_{n-k}(x_{k+1}, \dots, x_n) \\ &= \neg \text{NAE}_k(\neg x_1, \dots, \neg x_k) \wedge \text{AND}_{n-k}(x_{k+1}, \dots, x_n). \end{aligned}$$

Therefore,  $Q_E(f) < k + n - k = n$ .

**Case 2:**  $f_{x_1=0}(x) = \text{OR}_{n-1}((\neg)x_2, \dots, (\neg)x_n)$ . This means that we have two subcases.

**Case 2a:**  $f_{x_1=0}(x) = \text{OR}_{n-1}(\neg x_2, \dots, \neg x_n)$ . If  $g(y) = \text{AND}_{n-1}(x_2, \dots, x_n)$ , then

$$f(x) = (\neg x_1 \wedge \neg g(y)) \vee (x_1 \wedge g(y)) = x_1 \oplus g(y).$$

Therefore,  $Q_E(f) < n$ .

**Case 2b:**  $f_{x_1=0}(x) \neq \text{OR}_{n-1}(\neg x_2, \dots, \neg x_n)$ . Without loss of generality, we can suppose that  $f_{x_1=0}(x) = \text{OR}_{n-1}(x_2, (\neg)x_3, \dots, (\neg)x_n)$ , then let us query  $x_2$  first. If  $x_2 = 0$ , then  $f_{x_2=0}(x) = \neg x_1 \wedge \text{OR}_{n-2}((\neg)x_3, \dots, (\neg)x_n)$ . According to Theorem 5,  $Q_E(f_{x_2=0}) < n-1$ . If  $x_2 = 1$ , then  $f_{x_2=1}(x) = \neg x_1 \vee \text{AND}_{n-1}(x_1, x_3, \dots, x_n) = \neg x_1 \vee \text{AND}_{n-2}(x_3, \dots, x_n)$ . According to Theorem 5,  $Q_E(f_{x_2=1}) < n-1$ . According to Eq. (5),  $Q_E(f) < n-1+1 = n$ .

Now we need to consider the case that both  $f_{x_1=0}$  and  $f_{x_1=1}$  are  $\text{OR}_{n-1}$  functions. Without loss of generality, we assume that  $f_{x_1=1}(x) = \text{OR}_{n-1}(x_2, \dots, x_n)$ . This means that we have again two subcases.

**Case 3a:**  $f_{x_1=0}(x) = \text{OR}_{n-1}(x_2, \dots, x_n)$ . In this case, we have  $f(x) = \text{OR}_{n-1}(x_2, \dots, x_n)$  and  $Q_E(f) = n - 1 < n$ .

**Case 3b:**  $f_{x_1=0}(x) \neq \text{OR}_{n-1}(x_2, \dots, x_n)$ . Without loss of generality, let us suppose that there exists a  $k \in \{2, \dots, n\}$  such that  $f_{x_1=0}(x) = \text{OR}_{n-1}(\neg x_2, \dots, \neg x_k, x_{k+1}, \dots, x_n)$ . In such a case

$$f(x) = (\neg x_1 \wedge \text{OR}_{n-1}(\neg x_2, \dots, \neg x_k, x_{k+1}, \dots, x_n)) \vee (x_1 \wedge \text{OR}_{n-1}(x_2, \dots, x_n))$$

Let us query  $x_{k+1}$  to  $x_n$  first. If  $x_{k+1} = \dots = x_n = 0$ , let  $g(y) = f(x_1, \dots, x_k, 0, \dots, 0)$ , then

$$\begin{aligned} g(y) &= (\neg x_1 \wedge \text{OR}_{n-1}(\neg x_2, \dots, \neg x_k, )) \vee (x_1 \wedge \text{OR}_{n-1}(x_2, \dots, x_k)) \\ &= \text{NAE}_n(\neg x_1, x_2, \dots, x_k). \end{aligned}$$

Therefore,  $Q_E(g) < k$ . Otherwise, there exists a  $j \geq k + 1$  such that  $x_j = 1$ . It is now easy to show that  $f(x) = \neg x_1 \vee x_1 = 1$ . Therefore,  $Q_E(f) < n - k + k = n$ .

**Lemma 10.** *Let  $f : \{0, 1\}^n \rightarrow \{0, 1\}$  be a Boolean function. If there exist an  $i \in [n]$  such that  $f_{x_i=b}$  is equivalent to  $\text{AND}_{n-1}(\text{OR}_{n-1})$  up to some negations of the variables, then  $f_{x_j=c}$  is not equivalent to  $\text{OR}_{n-1}(\text{AND}_{n-1})$  up to some negations of the variables for  $j \neq i$ , where  $b, c \in \{0, 1\}$ .*

**Proof:** Without loss of generality, we assume that  $i = 1$ ,  $j = 2$  and  $f_{x_1=b}(x) = \text{AND}_{n-1}(x_2, \dots, x_n)$ . In such a case we have  $f(bc00 * \dots *) = f(bc01 * \dots *) = 0^3$ . If we fix  $c$ , then there are more than one inputs such that  $f_{x_2=c}(x) = 0$ . Therefore,  $f_{x_2=c}$  is not equivalent to  $\text{OR}_{n-1}$  up to some negations of the variables.

**Proof of Lemma 7:** According to Lemma 8, for every  $i \in [n]$ , there must exist a  $b_i \in \{0, 1\}$  such that  $f_{x_i=b_i}$  is isomorphic to  $\text{AND}_{n-1}$ , otherwise  $Q_E(f) < n$ . Without loss of generality, we assume that  $f_{x_1=b_1}$  is equivalent to  $\text{AND}_{n-1}(\text{OR}_{n-1})$  up to some negations of the variables. According to Lemma 10, no  $f_{x_i=b_i}$  is equivalent to  $\text{OR}_{n-1}(\text{AND}_{n-1})$  up to some negations of the variables. Therefore, for every  $i > 1$ ,  $f_{x_i=b_i}$  is equivalent to  $\text{AND}_{n-1}(\text{OR}_{n-1})$  up to some negations of the variables.

Now, suppose there exists  $c = c_1 \dots c_n \neq b$  for every  $i \in [n]$  such that  $f_{x_i=c_i}$  is equivalent to  $\text{AND}_{n-1}(\text{OR}_{n-1})$  up to some negations of the variables. Since  $c \neq b$ , there exist  $i \in [n]$  such that  $b_i \neq c_i$ . We have therefore that both  $f_{x_i=b_i}$  and  $f_{x_i=c_i}$  are isomorphic to  $\text{AND}_{n-1}$ . According to Lemma 9, we have  $Q_E(f) < n$ , which is a contradiction.

In order to make our main result easier to understand, we consider 4-bit Boolean functions first.

**Theorem 11.** *If  $f$  is a 4-bit Boolean function, then  $Q_E(f) = 4$  iff  $f$  is isomorphic to  $\text{AND}_4$ .*

**Proof:** If  $f$  is isomorphic to  $\text{AND}_4$ , then  $Q_E(f) = 4$  [19].

Assume that a 4-bit Boolean function  $f$  such that  $Q_E(f) = 4$ , we prove that  $f$  is isomorphic to  $\text{AND}_4$  as follows. According to Lemma 7, there exists one and only one  $b = b_1 b_2 b_3 b_4$  for every  $i \in [4]$  such that  $f_{x_i=b_i}$  is equivalent to  $\text{AND}_3(\text{OR}_3)$  up to some negations of the variables. Since for any 4-bit function  $f$  with  $b = b_1 b_2 b_3 b_4$ , there exists a function  $f'$  with  $b' = 0000$  isomorphic to  $f$ . We can get  $f'$  by some negations of the variables  $x_i$  whenever  $b_i = 1$ . Therefore, without loss of generality, we assume that  $b = 0000$  and for every  $i \in [4]$  such that  $f_{x_i=0}$  is equivalent to  $\text{OR}_3$  up to some negations of the variables.

Table 3: Values of 4-bit Boolean functions.

$x_1$	$x_2$	$x_3$	$x_4$	$f(x)$ : Case 1	Case 2	Case 3
0	0	0	0	0	1	1
0	0	0	1	1	1	1
0	0	1	0	1	1	*
0	0	1	1	1	1	*
0	1	0	0	1	1	1
0	1	0	1	1	1	1
0	1	1	0	1	1	1
0	1	1	1	1	0	1
1	0	0	0	1	1	1
1	0	0	1	1	1	1
1	0	1	0	1	1	1
1	0	1	1	1	0	1
1	1	0	0	1	1	*
1	1	0	1	1	0	*
1	1	1	0	1	0	*
1	1	1	1	*	*	*

There are three cases that we need now to consider:

**Case 1:** For every  $i \in [4]$ , there is no negation variable occurrence in  $f_{x_i=0}$ , that is  $f_{x_1=0}(x) = \text{OR}(x_2, x_3, x_4)$ ,  $f_{x_2=0}(x) = \text{OR}(x_1, x_3, x_4)$ ,  $f_{x_3=0}(x) = \text{OR}(x_1, x_2, x_4)$  and  $f_{x_4=0}(x) = \text{OR}(x_1, x_2, x_3)$ . See Case 1 in Table 3 for values of  $f(x)$ . We still do not the value of  $f(1111)$ . If  $f(1111) = 1$ , then  $f(x) = \text{OR}(x_1, x_2, x_3, x_4)$ , which is isomorphic to  $\text{AND}_4$ . If  $f(1111) = 0$ , then  $f(x) = \text{NAE}(x_1, x_2, x_3, x_4)$  and  $Q_E(f) < 4$ .

**Case 2:** There are negations of all variables in every  $f_{x_i=0}$ , that is  $f_{x_1=0}(x) = \text{OR}(\neg x_2, \neg x_3, \neg x_4)$ ,  $f_{x_2=0}(x) = \text{OR}(\neg x_1, \neg x_3, \neg x_4)$ ,  $f_{x_3=0}(x) = \text{OR}(\neg x_1, \neg x_2, \neg x_4)$  and  $f_{x_4=0}(x) = \text{OR}(\neg x_1, \neg x_2, \neg x_3)$ . See Case 2 in Table 3 for values of  $f(x)$ . If  $f(1111) = 1$ , then  $f(x) = \neg \text{Th}_4^3$  and  $Q_E(f) = 3 < 4$ . If  $f(1111) = 0$ , then  $f(x) = \neg \text{EXACT}_4^3$  and  $Q_E(f) = 3 < 4$ .

**Case 3:** There is an  $i \in [4]$  such that there is at least one negation variable occurrence and one no negation variable occurrence in  $f_{x_i=0}$ . Without loss of generality, we can now assume that  $f_{x_1=0}(x) = \text{OR}(x_2, \neg x_3, (\neg)x_4)$ . In order to analyse this case, we prove the following two lemmas first.

**Lemma 12.** *Let  $f$  be an  $n$ -bit Boolean function and  $f_{x_i=0}$  be equivalent to  $\text{OR}_{n-1}$  up to some negations of the variables for every  $i \in [n]$ . If  $f_{x_1=0}(x) = \text{OR}_{n-1}(x_2, \neg x_3, (\neg)x_4, \dots)$ , then  $f_{x_2=0}(x) = \text{OR}_{n-1}(x_1, \neg x_3, (\neg)x_4, \dots)$  and  $f_{x_3=0}(x) = \text{OR}_{n-1}(\neg x_1, \neg x_2, (\neg)x_4, \dots)$ .*

**Proof:** Since  $f_{x_1=0}(x) = \text{OR}_{n-1}(x_2, \neg x_3, (\neg)x_4, \dots)$ , there exists a  $y \in \{0, 1\}^{n-3}$  such that  $f(001y) = 0$ .

---

<sup>3\*</sup> will denote one bit that can be 0 or 1.

Table 4: Values of  $g(x_2, x_3, x_4)$ .

$x_2$	$x_3$	$x_4$	$g(x_2, x_3, x_4)$
0	0	0	1
0	0	1	1
0	1	0	*
0	1	1	*
1	0	0	*
1	0	1	*
1	1	0	*
1	1	1	*

Suppose that  $f_{x_2=0}(x) = \text{OR}_{n-1}(\neg x_1, (\neg)x_3, (\neg)x_4, \dots)$  or  $f_{x_2=0}(x) = \text{OR}_{n-1}((\neg)x_1, x_3, (\neg)x_4, \dots)$ . We have  $f(001y) = 1$ , which is a contradiction. Therefore,  $f_{x_2=0} = \text{OR}_{n-1}(x_1, \neg x_3, (\neg)x_4, \dots)$ .

Now suppose that  $f_{x_3=0}(x) = \text{OR}_{n-1}(x_1, (\neg)x_2, (\neg)x_4, \dots)$ . There have to exist  $c \in \{0, 1\}$  and  $z \in \{0, 1\}^{n-3}$  such that  $f(0c0z) = 0$ . Since  $f_{x_1=0}(x) = \text{OR}_{n-1}(x_2, \neg x_3, (\neg)x_4, \dots)$ , we have  $f(0c0z) = 1$ , which is a contradiction. Suppose that  $f_{x_3=0}(x) = \text{OR}_{n-1}((\neg)x_1, x_2, (\neg)x_4, \dots)$ . There exist  $c \in \{0, 1\}$  and  $z \in \{0, 1\}^{n-3}$  such that  $f(c00z) = 0$ . Since  $f_{x_2=0}(x) = \text{OR}_{n-1}(x_1, \neg x_3, (\neg)x_4, \dots)$ , we have  $f(c00z) = 1$ , which is a contradiction. Therefore,  $f_{x_3=0}(x) = \text{OR}_{n-1}(\neg x_1, \neg x_2, (\neg)x_4, \dots)$ .

**Lemma 13.** *Let  $f$  be an  $n$ -bit Boolean function. If there exist 4 distinct inputs  $x, y, u, v \in \{0, 1\}^n$  such that  $f(x) = f(y) = 1$  and  $f(u) = f(v) = 0$ , then  $f$  is not isomorphic to  $\text{AND}_n$ .*

**Proof:** If  $f$  is equivalent to  $\text{AND}_n$  up to some negations of the variables, then there exists just one  $x \in \{0, 1\}^n$  such that  $f(x) = 1$ . If  $f$  is equivalent to  $\text{OR}_n$  up to some negations of the variables, then there exists just one  $u \in \{0, 1\}^n$  such that  $f(u) = 0$ .

According to Lemma 12, we have  $f_{x_2=0}(x) = \text{OR}(x_1, \neg x_3, (\neg)x_4)$ , and  $f_{x_3=0}(x) = \text{OR}(\neg x_1, \neg x_2, (\neg)x_4)$ . See Case 3 in Table 3 for values of  $f(x)$ . It is easy to see that if  $x_1 \oplus x_2 = 1$ , then  $f(x) = 1$ . If  $x_1 \oplus x_2 = 0$ , then  $x_1 = x_2$  and  $f$  can be represented as a 3-bit Boolean function  $g(x_2, x_3, x_4)$ , see Table 4 for its values. Since  $f_{x_1=0}(x) = \text{OR}(x_2, \neg x_3, (\neg)x_4)$ , we have either  $g(010) = f(0010) = 0$  or  $g(011) = f(0011) = 0$ . Since  $f_{x_3=0}(x) = \text{OR}(\neg x_1, \neg x_2, (\neg)x_4)$ , we have either  $g(100) = f(1100) = 0$  or  $g(101) = f(1101) = 0$ . We also have  $g(000) = f(0000)$  and  $g(001) = f(0001) = 1$ . According to Lemma 13,  $g(x_2, x_3, x_4)$  is not isomorphic to  $\text{AND}_3$  and  $Q_E(g) < 3$ .

Now we give an exact quantum algorithm for  $f$  as follows:

- 1) Evaluate  $x_1 \oplus x_2$  with one query.
- 2) If  $x_1 \oplus x_2 = 1$ , then  $f(x) = 1$ .
- 3) If  $x_1 \oplus x_2 = 0$ , then  $f(x) = g(x_2, x_3, x_4)$ . Evaluate  $g$  with exact quantum algorithm.

Therefore, we have  $Q_E(f) < 1 + Q_E(g) < 1 + 3 = 4$ . The theorem has been proved.

Finally, we prove the most general case. The main idea of the proof is similar to the proof of the previous theorem.

**Theorem 14.** *If  $f$  is an  $n$ -bit Boolean function, then  $Q_E(f) = n$  iff  $f$  is isomorphic to  $AND_n$ .*

**Proof:** If  $f$  is isomorphic to  $AND_n$ , then  $Q_E(f) = n$  [19]. We prove the other direction by an induction on  $n$ .

**BASIS:** The result holds for  $n = 3$ .

**INDUCTION:** Suppose the result holds for  $n - 1$ , we will prove that the result holds for  $n$ . According to Lemma 7, there exists one and only one  $b = b_1 \dots b_n$  for every  $i \in [n]$  such that  $f_{x_i=b_i}$  is equivalent to  $AND_{n-1}$  ( $OR_{n-1}$ ) up to some negations of the variables. Without loss of generality, we assume that  $b = 0 \dots 0$  and for every  $i \in [n]$  such that  $f_{x_i=0}$  is equivalent to  $OR_{n-1}$  up to some negations of the variables.

There are three cases that we need to consider:

**Case 1:** For every  $i \in [n]$ , there is no negation variable occurrence in  $f_{x_i=0}$ , that is  $f_{x_i=0}(x) = OR_{n-1}(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$  for  $i \in [n]$ . It is easy to see that in such a case  $f(0 \dots 0) = 0$ ,  $f(1 \dots 1) = *$  and  $f(x) = 1$  for  $x \notin \{0 \dots 0, 1 \dots 1\}$ . If  $f(1 \dots 1) = 1$ , then  $f(x) = OR_n(x_1, \dots, x_n)$ , which is isomorphic to  $AND_n$ . If  $f(1 \dots 1) = 0$ , then  $f(x) = NAE(x_1, \dots, x_n)$  and  $Q_E(f) < n$ .

**Case 2:** There are all negation variable occurrences in every  $f_{x_i=0}$ , that is  $f_{x_i=0}(x) = OR_{n-1}(\neg x_1, \dots, \neg x_{i-1}, \neg x_{i+1}, \dots, \neg x_n)$  for  $i \in [n]$ . It is easy to see that  $f(x) = 1$  for  $|x| < n - 1$ ,  $f(x) = 0$  for  $|x| = n - 1$  and  $f(x) = *$  for  $|x| = n$ . If  $f(1 \dots 1) = 1$ , then  $f(x) = \neg Th_n^{n-1}$  and  $Q_E(f) = n - 1 < n$ . If  $f(1 \dots 1) = 0$ , then  $f(x) = \neg EXACT_n^{n-1}$  and  $Q_E(f) = n - 1 < n$ .

**Case 3:** There is an  $i \in [n]$  such that there is at least one negation variable occurrence and one no negation variable occurrence  $f_{x_i=0}$ . Without loss of generality, we assume that  $f_{x_1=0}(x) = OR(x_2, \neg x_3, (\neg)x_4, \dots)$ . According to Lemma 12, we have  $f_{x_2=0}(x) = OR(x_1, \neg x_3, (\neg)x_4, \dots)$  and  $f_{x_3=0}(x) = OR(\neg x_1, \neg x_2, (\neg)x_4, \dots)$ . For any  $y \in \{0, 1\}^{n-2}$ ,  $f(01y) = f(10y) = 1$ , that is  $f(x) = 1$  if  $x_1 \oplus x_2 = 1$ . If  $x_1 \oplus x_2 = 0$ , then  $x_1 = x_2$  and  $f$  can be represented as an  $(n - 1)$ -bit Boolean function  $g(x_2, \dots, x_n)$ . Since  $f_{x_1=0}(x) = OR(x_2, \neg x_3, (\neg)x_4, \dots)$ , there must exist a  $u \in \{0, 1\}^{n-3}$  such that  $f(001u) = g(01u) = 0$ . Since  $f_{x_3=0}(x) = OR(\neg x_1, \neg x_2, (\neg)x_4, \dots)$ , there must exist a  $v \in \{0, 1\}^{n-3}$  such that  $f(110v) = g(10v) = 0$ . We also have  $g(00 \dots 00) = f(000 \dots 00) = 1$  and  $g(00 \dots 01) = f(000 \dots 01) = 1$ . According to Lemma 13, we have that  $g(x_2, \dots, x_n)$  is not isomorphic to  $AND_{n-1}$  and  $Q_E(g) < n - 1$ .

Now we give an exact quantum algorithm for  $f$  as follows:

- 1) Evaluate  $x_1 \oplus x_2$  with one query.
- 2) If  $x_1 \oplus x_2 = 1$ , then  $f(x) = 1$ .
- 3) If  $x_1 \oplus x_2 = 0$ , then  $f(x) = g(x_2, \dots, x_n)$ . Evaluate  $g$  with exact quantum algorithm.

Therefore, we have  $Q_E(f) < 1 + Q_E(g) < 1 + n - 1 = n$ . The theorem has been proved.

**Corollary 15.** *Almost all  $n$ -bit Boolean functions can be computed by an exact quantum algorithm with less than  $n$  queries.*

**Proof:** It is easy to see that there are  $2 \times 2^n$   $n$ -bit Boolean functions which are isomorphic to  $AND_n$ . Since there are  $2^{2^n}$  Boolean functions on  $n$  variables, we see that the fraction of functions which have exact quantum query complexity  $n$  is  $o(1)$ . Thus almost all  $n$ -bit Boolean functions can be computed by an exact quantum algorithm with less than  $n$  queries.

## 7. Conclusion

We have first shown that  $\text{AND}_n$  is the only  $n$ -bit Boolean function in three special classes of Boolean functions, (including symmetric, monotone, read-once functions), up to isomorphism, that has exact quantum query complexity  $n$ . Finally, we have proved that in general  $\text{AND}_n$  is the only  $n$ -bit Boolean function, up to isomorphism, that has exact quantum query complexity  $n$ . This shows that the advantages for exact quantum query algorithms are more common than previously thought.

In the proof for special classes of Boolean functions, we have used their special properties of different types of Boolean functions. Each approach is different from each other. These approaches that we used in each type of Boolean functions may be helpful in analysis of exact quantum complexity for other interesting functions. In the approach for general case, we have used the properties of the true value table of the Boolean functions.

## Acknowledgements

The authors are thankful to the anonymous referees for their comments and suggestions on the early version of this paper. The third author would like to thank Alexander Rivosh for his help while visiting University of Latvia. Work of the first author was supported by FP7 FET projects QCS and QALGO and ERC Advanced Grant MQC (at the University of Latvia) and by National Science Foundation under agreement No. DMS-1128155 (at IAS, Princeton). Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation. Work of the second and third authors was supported by the Employment of Newly Graduated Doctors of Science for Scientific Excellence project/grant (CZ.1.07./2.3.00/30.0009) of Czech Republic.

## References

- [1] H. Buhrman and R. de Wolf (2002), *Complexity measures and decision tree complexity: a survey*, Theoretical Computer Science, 288, pp. 1–43, 2002.
- [2] L. K. Grover (1996), *A fast quantum mechanical algorithm for database search*, in Proceedings of 28th STOC, pp. 212–219. Also arXiv:9605043
- [3] A. Ambainis (2007), *Quantum walk algorithm for element distinctness*, SIAM Journal on Computing, 37, pp. 210–239. Also FOCS’04 and quant-ph/0311001.
- [4] A. Belovs (2012), *Span programs for functions with constant-sized 1-certificates*, in Proceedings of 43rd STOC, pp. 77–84. Also arXiv:1105.4024.
- [5] C. Dürr, M. Heiligman, P. Høyer, and M. Mhalla (2006), *Quantum query complexity of some graph problems*, SIAM Journal on Computing, 35, pp. 1310–1328. Earlier version in ICALP’04. Also arXiv:quant-ph/0401091.
- [6] P. W. Shor (1997), *Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer*, SIAM Journal on Computing, 26, pp. 1484–1509. Earlier version in FOCS’94. Also arXiv:9508027.
- [7] D. Simon (1997), *On the power of quantum computation*, SIAM Journal on Computing, 26, pp. 1474–1483. Earlier version in FOCS’94.
- [8] A. Ambainis and A. Yakaryılmaz (2012), *Superiority of exact quantum automata for promise problems*, Information Processing Letters, 112, pp. 289–291. Also arXiv:1101.3837.
- [9] G. Brassard and P. Høyer (1997), *An exact quantum polynomial-time algorithm for Simon’s problem*, in Proceedings of the Israeli Symposium on Theory of Computing and Systems, pp. 12–23. Also arXiv:9704027.
- [10] D. Deutsch and R. Jozsa (1992), *Rapid solution of problems by quantum computation*, in Proceedings of the Royal Society of London, volume A439, pp. 553–558.
- [11] J. Gruska, D.W. Qiu, and S.G. Zheng (2014), *Generalizations of the distributed Deutsch-Jozsa promise problem*, arXiv:1402.7254.



- [12] S.G. Zheng and D.W. Qiu (2014), *From quantum query complexity to state complexity*, arXiv:1407.7342.
- [13] J. Gruska, D.W. Qiu, and S.G. Zheng (2014), *Potential of quantum finite automata with exact acceptance*, arXiv:1404.1689.
- [14] S.G. Zheng, J. Gruska, and D.W. Qiu (2014), *On the state complexity of semi-quantum finite automata*, Theoretical Informatics and Applications 48, pp. 187–207. Earlier versions at LATA’14. Also arXiv:1307.2499.
- [15] R. Cleve, A. Eckert, C. Macchiavello, and M. Mosca (1998), *Quantum algorithms revisited*, in Proceedings of the Royal Society of London, volume A454, pp. 339–354. Also arXiv:9708016.
- [16] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser (1998), *A limit on the speed of quantum computation in determining parity*, Physical Review Letters, 81, pp. 5442–5444. Also arXiv:9802045.
- [17] A. Ambainis (2013), *Superlinear advantage for exact quantum algorithms*, in Proceedings of 45th STOC, pp. 891–900. Also arXiv:1211.0721.
- [18] A. Montanaro, R. Jozsa, and G. Mitchison (2013), *On exact quantum query complexity*, Algorithmica, DOI 10.1007/s00453-013-9826-8. Also arXiv:1111.0475.
- [19] R. Beals, H. Buhrman, R. Cleve, M. Mosca, and R. de Wolf (2001), *Quantum lower bounds by polynomials*, Journal of the ACM, 48, pp. 778–797. Earlier version in FOCS’98. Also arXiv:9802049.
- [20] J. Gruska (1999), *Quantum Computing*, McGraw-Hill (London).
- [21] M. Nielsen and I. Chuang (2000), *Quantum Computation and Quantum Information*, Cambridge University Press.
- [22] N. Nisan and M. Szegedy (1994), *On the degree of Boolean functions as real polynomials*, Computational Complexity, 4, pp. 301–313. Earlier version in STOC’92.
- [23] J. von zur Gathen and J. R. Roche (1997), *Polynomials with two values*, Combinatorica, 17, pp. 345–362.
- [24] T. Eiter, K. Makino, and G. Gottlob (2008), *Computational aspects of monotone dualization: A brief survey*, Discrete Applied Mathematics, 156, pp. 2035–2049.
- [25] H. Barnum and M. Saks (2004), *A lower bound on the quantum query complexity of read-once functions*, Journal of Computer and System Sciences, 69(2), pp. 244–258. Also arXiv:quant-ph/0201007.
- [26] M. Saks and A. Wigderson (1986), *Probabilistic Boolean decision trees and the complexity of evaluating game trees*, in Proceedings of FOCS’87, pp. 29–38.
- [27] M. Santha (1995), *On the Monte Carlo boolean decision tree complexity of read-once formulae*, Random Structures & Algorithms, 6(1), pp. 75–87.
- [28] A. Ambainis, A. Iraids, and J. Smotrovs (2013), *Exact quantum query complexity of EXACT and THRESHOLD*, in Proceedings of 8th TQC, pp. 263–269. Also arXiv:1302.1235.
- [29] S. Aaronson (2003), *Algorithms for Boolean function query properties*, SIAM Journal on Computing, 32, pp. 1140–1157. Also arXiv:cs/0107010.